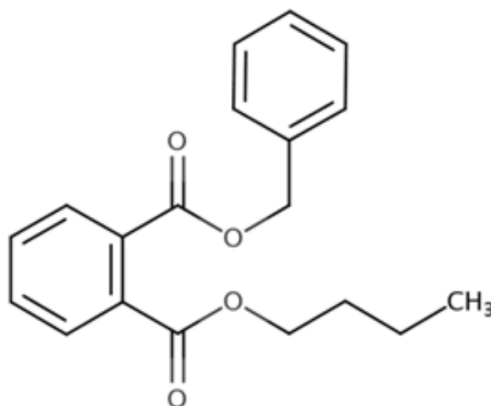


**Data Quality Evaluation and Data Extraction Information for
Physical and Chemical Properties for
Butyl benzyl phthalate (BBP)
(1,2-Benzenedicarboxylic acid, 1-butyl 2-(phenylmethyl) ester)**

Systematic Review Support Document for the Risk Evaluation

CASRN: 85-68-7



December 2025

This supplemental file contains information regarding the data extraction and evaluation results for data sources that were considered for the *Risk Evaluation for Butyl Benzyl Phthalate (BBP)* and that underwent systematic review. EPA used the TSCA systematic review process described in the *Draft Systematic Review Protocol Supporting TSCA Risk Evaluations for Chemical Substances* (also referred to as the '2021 Draft Systematic Review Protocol'). The systematic review steps are further described in the *Risk Evaluation for Butyl Benzyl Phthalate (BBP) – Systematic Review Protocol*. EPA conducted data extractions and data quality evaluations based on author-reported descriptions and results; additional analyses (*e.g.*, statistical analyses) potentially conducted by EPA are not contained in this supplemental file. Additionally, the overall quality determination (OQD) for each reference represents the data as a whole for each study and not for individual metric domains within a study.

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| Study Citation: | DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs. | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 3981013 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Results Value | liquid | | | |
| Results Details | not specified | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

| | |
|----------------------------------|--|
| Study Citation: | EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate. |
| OECD Harmonized Template: | Physical Form or State |
| HERO ID: | 1333728 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| CASRN and Test Material | 85-68-7; Butylbenzylphthalate |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; a clear, oily liquid; Not Reported |
| Results Value | a clear, oily liquid |
| Results Details | Not Reported |

| | | EVALUATION | |
|----------------------------|-----------|---|----------|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High |
| | Metric 2: | Appropriateness | High |
| | | | |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium |
| | Metric 4: | Reliability/Analytical Method | Medium |
| | | | |
| Domain 3: Other | Metric 5: | Databases | High |
| | Metric 6: | Models | N/A |

Overall Quality Determination

High

* Related References: From: Howard, P.H., S. Banerjee and K.H. Robillard. 1985. Measurement of water solubilities, octanol/water partition coefficients and vapor pressure of commercial phthalate esters. Environ. Toxicol. Chem. 4: 653–661. HERO ID 82189

| | |
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| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. |
| OECD Harmonized Template: | Physical Form or State |
| HERO ID: | 7325405 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR |
| Results Value | Liquid |
| Results Details | Not Reported |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|--|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; liquid; Not Reported | | | |
| Results Value | liquid | | | |
| Results Details | clear oily liquid w/slight characteristic odor and bitter taste | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; liquid; Not Reported | | | |
| Results Value | liquid | | | |
| Results Details | clear oily liquid w/slight characteristic odor and bitter taste | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 666726 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR Notes: NR | | | |
| Results Value | Clear, oily liquid | | | |
| Results Details | NR | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Citing HERO ID 5185266

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|---|--|---|------|--|
| Study Citation: | IPCS, (1999). Concise international chemical assessment document 17: Butyl benzyl phthalate. | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 675227 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; Not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; room temperature; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; liquid; Not Reported | | | |
| Results Value | clear, oily liquid | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Results Value | a clear, oily liquid with a slight odor and a bitter taste | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Value added under HSDB (2015) HEROID: 5926116

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|---|---|---|--------|--|
| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 678590 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; Butyl Benzyl Phthalate | | | |
| Confidentiality, Type, and Guideline | None; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; liquid; Not Reported | | | |
| Results Value | clear, slightly viscous liquid | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|---|--|---|----------|---|
| Study Citation: | Haynes, W. M. (2014). Butyl benzyl phthalate. :3-44. | | | |
| OECD Harmonized Template: | Physical Form or State | | | |
| HERO ID: | 5348395 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Results Value | liquid | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a recognized data collection where data are peer-reviewed by experts in the field. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Physical Form or State |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Results Value | liquid |
| Results Details | Not Reported |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|--|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available and peer-reviewed database. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 196.

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| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Physical Form or State |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Results Details | clear oil, liquid; slight odor |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available and peer-reviewed database. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Lewis, R.J. Sr. 2007. Hawley's Condensed Chemical Dictionary 15th Edition. John Wiley & Sons, Inc. New York, NY. P. 196.

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|---|---|---|----------|---|
| Study Citation: | DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs. | | | |
| OECD Harmonized Template: | Melting Point | | | |
| HERO ID: | 3981013 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Melting Point | -35 - °C | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; none | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Results Details Methods | not reported | | | |
| Standard Deviation Results | not reported | | | |
| Results Details | not reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

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| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. |
| OECD Harmonized Template: | Melting Point |
| HERO ID: | 7325405 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| Melting Point | < -35 °C |
| CASRN and Test Material | 85-68-7; Benzylbutyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR |
| Results Details Methods | not reported |
| Standard Deviation Results | not reported |
| Results Details | not reported |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|--|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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|---|--|---|----------|---|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Melting Point | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Melting Point | < -35 °C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Data measured for a structural analogue of the subject chemical substance are consistent with what is expected for the subject chemical substance structural properties, features or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

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|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Melting Point | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Melting Point | < -35 °C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

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| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | Melting Point |
| HERO ID: | 5926420 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Melting Point | -35 °C |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Results Details Methods | Measured conditions were not reported. |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

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|---|--|---|----------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. | | | |
| OECD Harmonized Template: | Melting Point | | | |
| HERO ID: | 666726 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Melting Point | < −35 °C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Results Details Methods | NR | | | |
| Standard Deviation Results | NR | | | |
| Results Details | NR | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Citing HERO ID 5185266

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Melting Point |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Melting Point | -35 °C |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Results Details Methods | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|--|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: David R.M. et al. 2012. Esters of Mono-, Di-, and Tricarboxylic Acids. Patty's Toxicology. 6th Ed. 199-2015. New York, NY: John Wiley & Sons, Inc.

| | |
|----------------------------------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. |
| OECD Harmonized Template: | Melting Point |
| HERO ID: | 1239592 |

| EXTRACTION | |
|---|---------------------------------|
| Parameter | Data |
| Melting Point | -35 °C |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR |
| Results Details Methods | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | Rating | | Comments |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

Medium

* Related References: Value added under HSDB (2015) HEROID: 5926116. Sax and Lewis (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

| | | | | |
|---|---|---|----------|--|
| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). | | | |
| OECD Harmonized Template: | Melting Point | | | |
| HERO ID: | 678590 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Melting Point | -40.5 - °C | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

| | | | | |
|---|--|---|----------|---|
| Study Citation: | CPSC, (2015). Exposure assessment: Composition, production, and use of phthalates. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5155508 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 - 377 C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | The data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with other physical properties. |
| | | | | |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| | | | | |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing peer-review. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| | | | | |
| Overall Quality Determination | | Medium | | |

* Related References: IARC (International Agency for Research on Cancer), 1982. IARC Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Some Industrial Chemicals and Dyestuffs. Vol. 29. International Agency for Research on Cancer. Lyon, France. Available at: <http://monographs.iarc.fr/ENG/Monographs/vol1-42/mono27.pdf>; HSDB (Hazardous Substances Data Bank). 2015. Hazardous Substances Data Bank online database, Toxnet Toxicology Data Network. U.S. National Library of Medicine. Available at: <http://toxnet.nlm.nih.gov/cgi-bin/sis/htmlgen?HSDB>.

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| Study Citation: | DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs. |
| OECD Harmonized Template: | Boiling Point |
| HERO ID: | 3981013 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| Boiling Point | 370 - C |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR |
| Standard Deviation Results | not reported |
| Results Details | @ 760 mm Hg |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|---|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

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|---|--|---|----------|--|
| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 7325405 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR | | | |
| Standard Deviation Results | not specified | | | |
| Results Details | at 10.10 hPa | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | Medium | Measured data are consistent with the subject chemical substance structural features; appears to be a typo in the reporting of vapor pressure value. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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|---|--|---|----------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 - C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | 10.10 hPa | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Low | The data are from an MSDS without known expert peer-review. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Bayer AG MSDS Extract concerning physico chemical properties of BBP.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 - C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | 10.10 hPa | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Low | The data are from an MSDS without known expert peer-review. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Bayer AG MSDS Extract concerning physico chemical properties of BBP.

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| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | Boiling Point |
| HERO ID: | 5926420 |

EXTRACTION

| Parameter | Data |
|---|----------------------------------|
| Boiling Point | 250 C |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Standard Deviation Results | Not Reported |
| Results Details | @ 22.5 torr |

EVALUATION

| Domain | Metric | Rating | Comments |
|----------------------------|---|--------|--|
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination**High**

* Related References: Haertel, Georg H.; Journal of Chemical and Engineering Data; vol. 30; nb. 1; (1985); p. 57 - 61

| | | | | |
|---|--|---|----------|--|
| Study Citation: | Haynes, W. M. (2014). Butyl benzyl phthalate. :3-44. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5348395 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a peer-reviewed data collection. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 666726 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Standard Deviation Results | NR | | | |
| Results Details | NR | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Citing HERO ID 5185266

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Boiling Point |
| HERO ID: | 5926116 |

EXTRACTION

| Parameter | Data |
|---|----------------------------------|
| Boiling Point | 370 C |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

EVALUATION

| Domain | Metric | Rating | Comments |
|----------------------------|---|--------|--|
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination**High**

* Related References: Haynes, W.M. 2014. CRC Handbook of Chemistry and Physics. 95th Edition. CRC Press LLC, Boca Raton: FL.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Value added under HSDB (2015) HEROID: 5926116. Sax and Lewis (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

| | |
|----------------------------------|---|
| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). |
| OECD Harmonized Template: | Boiling Point |
| HERO ID: | 678590 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Boiling Point | 370 - C |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | None; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

Medium

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

| | | | | |
|---|---|---|----------|---|
| Study Citation: | Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 679796 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Standard Deviation Results | NR | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Biosynth

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|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: LabNetwork

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|---|---|---|----------|---|
| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5926148 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Alfa Aesar

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|---|---|---|----------|--|
| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5926148 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available database that provides references to the original, peer-reviewed source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: PhysProp

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|---|---|---|----------|---|
| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5926148 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Alfa Aesar

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|---|---|---|----------|---|
| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. | | | |
| OECD Harmonized Template: | Boiling Point | | | |
| HERO ID: | 5926148 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Boiling Point | 370 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Biosynth

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|---|--|---|----------|---|
| Study Citation: | Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 1322045 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.119 g/mL | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Density Type | Not Reported | | | |
| System | Not Reported | | | |
| Temperature | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased toward a particular outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a peer-reviewed secondary source without inclusion of references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|---|---|---|--------|---|
| Study Citation: | DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 3981013 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.116 - | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Density Type | specific gravity (density of a substance divided by the density of water) | | | |
| System | not specified | | | |
| Temperature | 25°C | | | |
| Standard Deviation Results | not reported | | | |
| Results Details | not reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

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|----------------------------------|--|
| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. |
| OECD Harmonized Template: | Density |
| HERO ID: | 7325405 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| Density | 1.116 g/cm3 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR |
| Density Type | relative density |
| System | not specified |
| Temperature | 20°C |
| Standard Deviation Results | not specified |
| Results Details | not specified |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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|---|--|---|----------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.114 - 1.122 g/cm3 | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Density Type | density | | | |
| System | Not Reported | | | |
| Temperature | 25°C | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.114 - 1.122 g/cm3 | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Density Type | density | | | |
| System | Not Reported | | | |
| Temperature | 25°C | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Monsanto internal data (1988); Santicizer 160 bulletin. Monsanto Europe S.A., 8th edition.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 666726 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.1 g/cm3 | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Density Type | density | | | |
| System | NR | | | |
| Temperature | 25°C | | | |
| Standard Deviation Results | NR | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Citing HERO ID 5185266

| | | | | |
|---|--|---|----------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 666726 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 10.8 | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Density Type | relative vapor density | | | |
| System | NR | | | |
| Temperature | Not Reported | | | |
| Standard Deviation Results | NR | | | |
| Results Details | Air=1 | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Citing National Toxicology Program (1991) NTP Chemical Repository Data Sheet: Butyl BenzylPhthalate, Research Triangle Park, NC.

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|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.116 | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Density Type | specific gravity | | | |
| System | NA | | | |
| Temperature | 25°C | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Sax and Lewis (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 10.8 | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Density Type | vapor density | | | |
| System | NA | | | |
| Temperature | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Value added under HSDB (2015) HEROID: 5926116

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|---|---|---|----------|--|
| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 678590 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.12 - | | | |
| CASRN and Test Material | 85-68-7; Butyl Benzyl Phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Density Type | Specific Gravity | | | |
| System | Not Reported | | | |
| Temperature | NR | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

| | |
|----------------------------------|---|
| Study Citation: | Park, C., Sheehan, R. J. (2000). Phthalic acids and other benzenepolycarboxylic acids. :1-45. |
| OECD Harmonized Template: | Density |
| HERO ID: | 679796 |

| EXTRACTION | |
|---|--------------------------------------|
| Parameter | Data |
| Density | 1.111 |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | None; experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR |
| Density Type | density reported as specific gravity |
| System | NR |
| Temperature | 25 deg C |
| Standard Deviation Results | NR |
| Results Details | Not Reported |

| | | EVALUATION | | |
|----------------------------|-----------|---|--------|---|
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

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|---|--|---|--------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.119 g/mL | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; experimental; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Density Type | density | | | |
| System | not specified | | | |
| Temperature | 20°C | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Cites: Merck Millipore

| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
|---|--|---|----------|---|
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.121 g/mL | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; experimental; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Density Type | density | | | |
| System | not specified | | | |
| Temperature | 4°C | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Cites: Merck Millipore

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|---|--|---|--------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.1 g/mL | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; experimental; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Density Type | density | | | |
| System | not specified | | | |
| Temperature | Not reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Cites: Alfa Aesar

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|----------------------------------|--|
| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | Density |
| HERO ID: | 5926420 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Density | 1.118 g/cm3 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 20°C |
| Standard Deviation Results | Not Reported |
| Results Details | 20°C; 2 values were reported in Reaxys; 1 value was reported as 1.118 at 20°C; 1 value was at unreported temperatures. |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Haertel, Georg H.; Journal of Chemical and Engineering Data; vol. 30; nb. 1; (1985); p. 57 - 61

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| Study Citation: | Haynes, W. M. (2014). Butyl benzyl phthalate. :3-44. |
| OECD Harmonized Template: | Density |
| HERO ID: | 5348395 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Density | 1.119 g/cm3 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 25°C |
| Standard Deviation Results | Not Reported |
| Results Details | 25°C |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a recognized, peer-reviewed data collection. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Density |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Density | 1.119 g/cm3 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 25°C |
| Standard Deviation Results | Not Reported |
| Results Details | 25°C |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a publicly available, peer-reviewed database that provides references to a peer-reviewed data collection. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Haynes, W.M. (Ed.) 2014. CRC Handbook of Chemistry and Physics. 95th edition. CRC Press LLC, Boca Raton: FL.

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|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Density | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Density | 1.1 g/cm3 | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Alfa Aesar

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Density |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|-----------------------------------|
| Parameter | Data |
| Density | 10.8 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| System | Not reported |
| Temperature | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | air = 1 |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a publicly available, peer-reviewed database that provides references to original sources. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Lewis, R.J., Sr. (Ed.) 2012. Sax's Dangerous Properties of Industrial Materials. 12th edition. Wiley-Interscience, Wiley & Sons, Inc. Hoboken, NJ. P. 501

| | | | | |
|---|--|---|----------|--|
| Study Citation: | California Office of Environmental Health Hazard Assessment (OEHHA) (2013). Evidence on the carcinogenicity of butyl benzyl phthalate. | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 5155605 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 8.55E-6 mm Hg | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | 20°C | | | |
| System | NR | | | |
| Standard Deviation Results | NR | | | |
| Results Details | NR | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: No source cited; however, a similar value (8.6E-6 mm Hg) was reported in HERO IDs 1239592 and 5155508.

| | | | | |
|---|--|---|----------|---|
| Study Citation: | Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43. | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 1322045 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 2.49x10-3 Pa | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | 25°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased toward a particular outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a peer-reviewed secondary source without inclusion of references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|---|---|---|--------|---|
| Study Citation: | DOE, (2016). Table 1: Chemicals of concern and associated chemical information. PACs. | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 3981013 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 8.25x10-6 - mm Hg | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Temperature | 25°C | | | |
| System | not reported | | | |
| Standard Deviation Results | not reported | | | |
| Results Details | not reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review; specific source not reported. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: primary reference not specified but include CRC (2009), HSDB (no date), Merck (2006), SAX (2012)

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|----------------------------------|--|
| Study Citation: | EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 1333728 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Vapor Pressure | 1.15 mPa |
| CASRN and Test Material | 85-68-7; Butylbenzylphthalate |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported |
| Temperature | 20C |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: From: Gledhill, W.E., R.G. Kaley, W.J. Adams, O. Hicks, P.R. Michael and V.W. Saeger. 1980. An environmental safety assessment of butylbenzyl phthalate. Environ. Sci. Technol. 14: 301–305. [no HERO ID]

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| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 7325405 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| Vapor Pressure | 0.00112 Pa |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR |
| Temperature | 20°C |
| System | not specified |
| Standard Deviation Results | not specified |
| Results Details | not specified |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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|---|--|--------|--|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.00004 Pa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; extrapolated; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. | |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. | |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. | |
| | Metric 4: Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. | |
| Domain 3: Other | Metric 5: Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. | |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. | |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Bayer AG (1987) Dampfdruckbestimmung von Unimol BB. Bayer AG, Leverkusen, den 07.11.87.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.00799 Pa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 25°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Mabey W.R. and T. Mill (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. J. Phys. Chem. Ref. Data 7, 383-415. HERO ID 9848.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.5066 Pa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; experimental; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Low | The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Low | | |

* Related References: Citing Bayer-Denmark in Monsanto (1988)

| | | | | |
|---|--|---------------|--|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.00004 Pa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; extrapolated; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. | |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. | |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. | |
| | Metric 4: Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. | |
| Domain 3: Other | Metric 5: Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. | |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. | |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Bayer AG (1987) Dampfdruckbestimmung von Unimol BB. Bayer AG, Leverkusen, den 07.11.87.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.00799 Pa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 25°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Mabey W.R. and T. Mill (1978) Critical review of hydrolysis of organic compounds in water under environmental conditions. J. Phys. Chem. Ref. Data 7, 383-415. HERO ID 9848.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.5066 Pa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; experimental; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Low | The data are from a primary source without expert peer-review or an unknown secondary source without peer-review and references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Low | | |

* Related References: Citing Bayer-Denmark in Monsanto (1988)

| | |
|----------------------------------|--|
| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 5926420 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Vapor Pressure | 1.50015E-6 - 9.1E-5 mm Hg |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 25°C |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | 5 data points were reported in Reaxys; 4 values were reported at 1.50015E-6 to 9.1E-5 torr at standard temperature; 1 data point was outside the range, measured at non-standard or unreported temperatures. |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Data range determined from multiple primary sources in REAXYS.

| | |
|----------------------------------|---|
| Study Citation: | Gobble, C., Chickos, J., Verevkin, S. P. (2014). Vapor pressures and vaporization enthalpies of a series of dialkyl phthalates by correlation gas chromatography. Journal of Chemical and Engineering Data 59(4):1353-1365. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 5433544 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Vapor Pressure | 2.0E-4 Pa |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | No; Aldrich; NR; Mass fraction: 0.99 Notes: Analytical standard: EPA 606-M phthalate ester mix. Source: Supelco. |
| Temperature | 298.15 K |
| System | Correlation Gas Chromatography |
| Standard Deviation Results | Not specified; however, uncertainties in results were evaluated |
| Results Details | liquid phase vapor pressure. Manuscript authors erroneously omitted "-" from superscript in Table 19: "p·10 ⁶ /Pa" should be written as "p·10 ⁻⁶ /Pa". Same issue with Table 22. |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | This metric is not applicable to this type of study. |

Overall Quality Determination

High

| | |
|----------------------------------|---|
| Study Citation: | Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 679985 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Vapor Pressure | 1.1E-3 Pa |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; If more than one manufacturer produced the individual PAE, the PAE product provided to us was an equal-proportion blend. |
| Radiolabel, Source, State, and Purity | NR; Provided to Chemical Manufacturers' Association by U.S. manufacturers.; NR; Each sample contained less than 1 % of non-PAE material, as determined by another laboratory. Notes: single isomer |
| Temperature | 25°C |
| System | Measured by the gas saturation method: U.S. Environmental Protection Agency. 1980. Environmental test standards: Proposed rules. Vapor pressure. Fed. Reg. 45:77345-77350. |
| Standard Deviation Results | 0.1E-3 |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) and other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | Peer-reviewed journal article with results compared to other literature values. |
| | Metric 4: | Reliability/Analytical Method | High | Standard method used with experimental details reported. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

| | | | | |
|---|--|---|----------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 666726 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 1.14 mPa | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Temperature | 20°C | | | |
| System | NR | | | |
| Standard Deviation Results | NR | | | |
| Results Details | NR | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Verschueren, 1996 HERO ID 5185266

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|---|--|---|----------|--|
| Study Citation: | IPCS, (1999). Concise international chemical assessment document 17: Butyl benzyl phthalate. | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 675227 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 0.1 - Pa | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; Not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | Medium | Measured data are higher than expected for the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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| Study Citation: | Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 5433285 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Vapor Pressure | 0.014 - 23.8 Pa |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate-BBP |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | None; NR; NR; NR |
| Radiolabel, Source, State, and Purity | None; NR; NR; 0.98 (Supplier purity) Notes: Purity checked by GC >0.99 |
| Temperature | 343.15 K to 423.15 K |
| System | Test method: gas saturation method in absolute mode. |
| Standard Deviation Results | 0.0005-0.45 |
| Results Details | Several sources of uncertainty noted in using the saturation apparatus, especially for BBP with its very low vapor pressure. |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | Medium | Measured data are consistent with the subject chemical substance structural features. Not measured/reported for standard temperature. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is likely to be appropriate based on comparison with peer-reviewed sources. Sources of uncertainty are noted in measuring very low vapor pressure. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

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| Study Citation: | Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 807140 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| Vapor Pressure | 1.27X10 ⁻³ Pa |
| CASRN and Test Material | 85-68-7; butylbenzyl phthalate |
| Confidentiality, Type, and Guideline | none; QSAR; Quantitative Structure-Property relationship model for estimation of solubility in air |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: BBzP |
| Temperature | Not Reported |
| System | Predictive model developed using gas law: $S(A) = P(\text{liquid substance})/RT$ where R= gas constant (8.314 Pa m ³ mol ⁻¹ K ⁻¹) and T = absolute temperature (298K); Log S(A) = -0.2324 - 0.3215 (Lu) |
| Standard Deviation Results | Not Reported |
| Results Details | Log S(A): n = 15; correlation coefficient (R) = 0.9461; standard error (SE) = 0.27; leave-one-out cross validation correlation coefficient (Rsv) = 0.9218; corresponding standard errors (scv) = 0.34 |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | High | The model had a defined, unambiguous endpoint AND the model performance was known and r ² > 0.7, q ² > 0.5, and SE < 0.3 (ECHA, 2016). |

Overall Quality Determination

High

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| Study Citation: | NIST, (2022). NIST Chemistry WebBook. Benzyl butyl phthalate (85-68-7). Standard Reference Database No. 69. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 10225222 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Vapor Pressure | Not Reported |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | No; calculation; Calculated from the vapor pressure data reported by the method of least squares |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR |
| Temperature | 431 K |
| System | NR |
| Standard Deviation Results | NR |
| Results Details | Enthalpy of vaporization = $\Delta v_{\text{apH}} = 89.0$ kJ/mol. Based on data from 416-516 K. |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|--|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Citing Stephenson, Richard M.; Malanowski, Stanislaw, Handbook of the Thermodynamics of Organic Compounds, 1987, <https://doi.org/10.1007/978-94-009-3173-2>.

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Vapor Pressure | 8.25E-6 mm Hg |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 25°C |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a publicly available, peer-reviewed database that provides references to original sources. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

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| Overall Quality Determination | High |
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* Related References: Howard, P.H. et al. 1985. Environ Tox Chem 4: 653-61.

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|---|--|---------------|--|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 8.6X10-6 mm Hg | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | NA | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. | |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. | |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. | |
| | Metric 4: Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. | |
| Domain 3: Other | Metric 5: Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. | |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. | |
| Overall Quality Determination | | Medium | | |

* Related References: Verschueren, (1983) (page missing from document); Hawley's, (1987). 11th ed. (N.I. Sax and R.J. Lewis, Sr., Eds.), p. 184. Van Nostrand Reinhold, New York.; Sax and Lewis, (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

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| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). | | | |
| OECD Harmonized Template: | Vapor Pressure | | | |
| HERO ID: | 678590 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Vapor Pressure | 6x10^-7 - mm Hg | | | |
| CASRN and Test Material | 85-68-7; Butyl Benzyl Phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 25°C | | | |
| System | NR | | | |
| Standard Deviation Results | NA | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

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| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. |
| OECD Harmonized Template: | Vapor Pressure |
| HERO ID: | 5926148 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Vapor Pressure | 8.25E-6 mm Hg |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | Not Reported |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a publicly available database that provides references to original sources. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: PhysProp. Howard, PH et al. 1985

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|---|--|---|----------|---|
| Study Citation: | Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 1322045 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k _{ow} | 4.70 | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | 25°C | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased toward a particular outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a peer-reviewed secondary source without inclusion of references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|----------------------------------|--|
| Study Citation: | EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 1333728 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| log k_{ow} | 4.9 |
| CASRN and Test Material | 85-68-7; Butylbenzylphthalate |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported |
| Temperature | Not Reported |
| System | Not Reported |
| pH | Not Reported |
| Results Details Method | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|---|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors. |
| | Metric 2: | Appropriateness | High | |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| | Metric 4: | Reliability/Analytical Method | Medium | |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | N/A | |

Overall Quality Determination

High

* Related References: From: Leyder, F. and P. Boulanger. 1983. Ultraviolet absorption, aqueous solubility, and octanol–water partition coefficient for several phthalates. Bull. Environ. Contam. Toxicol. 30: 152–157. [no HERO ID]

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|---|--|---|----------|--|
| Study Citation: | EC/HC, (2017). Draft screening assessment: Phthalate substance grouping. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 5353181 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k_{ow} | 4.91 | | | |
| CASRN and Test Material | 85-68-7; Dibutyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; experimental; not specified | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | not specified | | | |
| System | not specified | | | |
| pH | not specified | | | |
| Results Details Method | not specified | | | |
| Standard Deviation Results | not specified | | | |
| Results Details | not specified | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Source cited: ECHA c2007-2015b

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| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 7325405 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| log k_{ow} | 4.84 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR |
| Temperature | not specified |
| System | not specified |
| pH | not specified |
| Results Details Method | not specified |
| Standard Deviation Results | not specified |
| Results Details | not specified |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 5926420 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| log k_{ow} | 4.77 - 4.84 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | Not Reported |
| System | Not Reported |
| pH | Not Reported |
| Results Details Method | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | @ 25 C; 4 values were reported in Reaxys; 2 values were reported in the range of 4.77 to 4.84 at 25 C; 2 values were reported at unreported temperatures. |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

| | | | | |
|---|--|---|----------|--|
| Study Citation: | Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 679985 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log <i>k_{ow}</i> | 3.57 | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; If more than one manufacturer produced the individual PAE, the PAE product provided to us was an equal-proportion blend. | | | |
| Radiolabel, Source, State, and Purity | NR; Provided to Chemical Manufacturers' Association by U.S. manufacturers.; NR; Each sample contained less than 1 % of non-PAE material, as determined by another laboratory. Notes: single isomer | | | |
| Temperature | Not reported | | | |
| System | HPLC method from a draft ASTM standard practice: Swann, R.L., D.A. Laskowski, P.J. McCall, K. Vander Kuy and H.J. Dishburger. 1983. Residue Rev. 85:17-28. | | | |
| pH | Not reported | | | |
| Results Details Method | The standards were benzene (log KOW=2.13), bromobenzene (log KOW = 2.99), biphenyl (log KO, = 3.76), bibenzyl (log KOW = 4.81), p,p-DDE (log KOW = 5.69), 2,4,5,2',5'-pentachlorobiphenyl (log KOW = 6.11) and 2,4,5,2',4',5'-hexachlorobiphenyl (log KOW = 6.72). | | | |
| Standard Deviation Results | 0 | | | |
| Results Details | Result is noted as being a log unit lower than other literature values. | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|----------------------------------|--|
| Study Citation: | IARC, (1999). Some chemicals that cause tumours of the kidney or urinary bladder in rodents and some other substances. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 666726 |

| EXTRACTION | |
|---|---------------------------------|
| Parameter | Data |
| log k_{ow} | 4.91 - |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; not specified; NR |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR |
| Temperature | NR |
| System | NR |
| pH | NR |
| Results Details Method | NR |
| Standard Deviation Results | NR |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|---|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate OR the analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Citing HERO ID 5185266

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| Study Citation: | Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 5433285 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| log k_{ow} | 4.58 |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate-BBP |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | None; NR; NR; NR |
| Radiolabel, Source, State, and Purity | None; NR; NR; 0.98 (Supplier purity) Notes: Purity checked by GC >0.99 |
| Temperature | 298.15 K |
| System | Test method: static mode by using the shake-flask method. Volume proportion of octanol/water=1/8 for BBP. |
| pH | Not reported |
| Results Details Method | HPLC-UV; internal standard: dibutyl phthalate |
| Standard Deviation Results | Not Reported |
| Results Details | Measured at atmospheric pressure 0.1MPa (ca. 750 mm Hg); |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | Author reported the value is in good agreement (1-3.6% deviation) with two reported values and less so (11.4-15.3% deviation) with two reported values. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination
High

| | | | | |
|---|--|---|---------------|---|
| Study Citation: | Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 807140 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k_{ow} | 5.22 | | | |
| CASRN and Test Material | 85-68-7; butylbenzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; QSAR; Quantitative Structure-Property relationship model for estimation of log Kow | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: BBzP | | | |
| Temperature | not applicable | | | |
| System | QSPR model using the Lu index, which is based on the shortest distance matrix. | | | |
| pH | not applicable | | | |
| Results Details Method | Predictive model developed using Lu index: Log Kow = -4.7875 + 0.5315 (Lu) | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | n = 15; correlation coefficient (R) = 0.9836; standard error (SE) = 0.40; leave-one-out cross validation correlation coefficient (Rsv) = 0.9784; corresponding standarderrors (scv) = 0.47 | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | Uninformative | The QSPR model failed the standard error threshold of <0.3 and is therefore rated unacceptable. |
| Overall Quality Determination | | Medium | | |

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|---|--|---|----------|--|
| Study Citation: | Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 654554 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k _{ow} | 4.87 | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Calculation; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not reported | | | |
| System | Not reported | | | |
| pH | Not reported | | | |
| Results Details Method | Not reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | calculated Pow-values -MedChem-Software 1989 | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | Medium | Calculated data consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear. |
| | Metric 4: | Reliability/Analytical Method | N/A | This matrix is not applicable to this calculated data. |
| Domain 3: Other | Metric 5: | Databases | N/A | This matrix is not applicable to this calculated data. |
| | Metric 6: | Models | High | The model had a defined, unambiguous endpoint and the model performance was known. |
| Overall Quality Determination | | High | | |

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| log k_{ow} | 4.73 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | Not Reported |
| System | Not Reported |
| pH | Not Reported |
| Results Details Method | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available database that provides references to a peer-reviewed source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Ellington, J.J.; Floyd, T.L.. 1996. Octanol/water partition coefficients for eight phthalate esters. EPA/600/S-96/006. Athens, GA: USEPA, National Exposure Research Lab.

| | |
|----------------------------------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. |
| OECD Harmonized Template: | logKow |
| HERO ID: | 1239592 |

| EXTRACTION | |
|---|---------------------------------|
| Parameter | Data |
| log k_{ow} | 4.77 |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR |
| Temperature | Not Reported |
| System | Not Reported |
| pH | Not Reported |
| Results Details Method | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

Medium

* Related References: HEROID: 1337260 Gledhill et al (1980). An environmental safety assessment of butyl benzyl phthalate. Environ. Sci. Technol. 14, 301-305

| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
|---|--|---|----------|--|
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k_{ow} | 4.91 | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: HEROID: 679764 Leyder and Boulanger (1983). Ultraviolet absorption, aqueous solubility, and octanol-water partition for several phthalates. Bull. Environ. Contam. Toxicol. 30, 152-157.

| | | | | |
|---|---|---|--------|--|
| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 678590 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k_{ow} | 4.59 - | | | |
| CASRN and Test Material | 85-68-7; Butyl Benzyl Phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

| | | | | |
|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log <i>k_{ow}</i> | 3.388 | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: LabNetwork

| | | | | |
|---|---|---|----------|--|
| Study Citation: | SRC, (1984). Final report measurement of octanol-water partition coefficients of phthalate esters. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 1316207 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k _{ow} | 3.57 - | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; experimental; HPLC method | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; US Manufacturers; Not Reported; Not Reported Notes: analyzed to be within commercial specification limits | | | |
| Temperature | 25°C | | | |
| System | partition coefficient correlated to HPLC retention time | | | |
| pH | Not reported | | | |
| Results Details Method | HPLC | | | |
| Standard Deviation Results | 0 | | | |
| Results Details | Author states the value is lower than most of the other reported or calculated values. | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | Low | Calculated value is lower than expected. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|---|---|---|--------|--|
| Study Citation: | U.S. EPA, (2017). Original BAF and BCF Data. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 3970058 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k_{ow} | 4.73 | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Not specified; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR | | | |
| Temperature | NR | | | |
| System | NR | | | |
| pH | NR | | | |
| Results Details Method | NR | | | |
| Standard Deviation Results | NR | | | |
| Results Details | Mean log kow of 4.73 also reported as a calculated value. | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing HSDB (no year)

| | | | | |
|---|---|---|----------|--|
| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. | | | |
| OECD Harmonized Template: | logKow | | | |
| HERO ID: | 5926148 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| log k_{ow} | 4.73 | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available database that references peer-reviewed original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: PhysProp. Ellington, JT and Floyd, TL. 1996

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|---|---|---|----------|--|
| Study Citation: | Analytical Bio-Chemistry Labs, (1986). ABC final report - Method validation and water solubility for butyl benzyl phthalate analysis in well water. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1359224 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.5 - 2.8 ppm | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; room temp; NR | | | |
| Radiolabel, Source, State, and Purity | NR; Monsanto Co; Liquid; 100% | | | |
| Temperature | 15-20°C | | | |
| System | Solubility in well water, sampling date 4/2/1985, 700 ft well at ABC Laboratories; devoid of O2 therefore passed through aeration reservoir | | | |
| pH | 7.8-8.3 | | | |
| Results Details Method | Solubility in well water with a hardness of 250 mg/L at a temp of 15 deg C = 2.6 ppm | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|---|
| Study Citation: | Boese, B. L. (1984). Uptake efficiency of the gills of english sole (parophrys vetulus) for 4 phthalate esters. Canadian Journal of Fisheries and Aquatic Sciences 41(11):1713-1718. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1316095 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 1.9 mg/L | | | |
| CASRN and Test Material | 85-68-7; BBP | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | 12°C | | | |
| System | Column generator method; seawater pumped through a sand column with the test substance. | | | |
| pH | Not reported | | | |
| Results Details Method | Extraction conducted with C18 Bond-Elut columns and eluted with ethylacetate, prior to electron capture capillary gas chromatography analysis. | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Determined for 25 o/oo seawater | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) and/or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | Methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytic method is non-standard but is expected to be appropriate. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

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|---|--|---|----------|---|
| Study Citation: | Cao, X. L. (2010). Phthalate esters in foods: Sources, occurrence, and analytical methods. Comprehensive Reviews in Food Science and Food Safety 9(1):21-43. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1322045 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 3.8 mg/L | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | 25°C | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased toward a particular outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a peer-reviewed secondary source without inclusion of references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

| Study Citation: | EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate. | | | |
|---|--|--|--------|--|
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1333728 | | | |
| EXTRACTION | | | | |
| Parameter | | Data | | |
| Water Solubility | | 2.69 mg/L | | |
| CASRN and Test Material | | 85-68-7; Butylbenzylphthalate | | |
| Confidentiality, Type, and Guideline | | no; not specified; Not Reported | | |
| Solvent, Reactivity, Storage, and Stability | | water; Not Reported; Not Reported; Not Reported | | |
| Radiolabel, Source, State, and Purity | | Not Reported; Not Reported; Not Reported; Not Reported | | |
| Temperature | | 25C | | |
| System | | Not Reported | | |
| pH | | Not Reported | | |
| Results Details Method | | Not Reported | | |
| Standard Deviation Results | | Not Reported | | |
| Results Details | | Not Reported | | |
| EVALUATION | | | | |
| Domain | | Metric | Rating | Comments |
| Domain 1: Substance | | | | |
| | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors. |
| Domain 2: Test Reliability | | | | |
| | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | | | | |
| | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | | High | |

* Related References: From: Howard, P.H., S. Banerjee and K.H. Robillard. 1985. Measurement of water solubilities, octanol/water partition coefficients and vapor pressure of commercial phthalate esters. Environ. Toxicol. Chem. 4: 653–661. [HERO ID: 82189]

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| Study Citation: | EC/HC, (2017). Draft screening assessment: Phthalate substance grouping. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 5353181 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69 mg/L | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| Temperature | not specified | | | |
| System | not specified | | | |
| pH | not specified | | | |
| Results Details Method | not specified | | | |
| Standard Deviation Results | not specified | | | |
| Results Details | not specified | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Source cited: ECHA c2007-2015b

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|---|---|---|--------|--|
| Study Citation: | ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 679967 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.9E3 ug/L | | | |
| CASRN and Test Material | Not Reported; BBP | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Data are measured or estimated for the subject chemical substance. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Hirzy, J.W., Adams, W.J., Gledhill, W.E. and Mieuse, J.P. (1979). Phthalates esters: the environmental issues. Unpublished document, Monsanto Industrial Chemicals Co. No HERO ID.

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|---|---|---|----------|--|
| Study Citation: | ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 679967 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.82E3 ug/L | | | |
| CASRN and Test Material | Not Reported; BBP | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 20 deg C | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Leyder and Boulanger (1983) HERO ID 679764.

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|---|---|---|----------|--|
| Study Citation: | ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 679967 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69E3 ug/L | | | |
| CASRN and Test Material | Not Reported; BBP | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 25 deg C | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing CMA (1983). Measurement of the water-solubility of phthalate esters. Final report, Contract PE-11. 0-WS-SRL. LI533-06, Syracuse Res. Corp., April, 1983. No HERO ID.

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|---|---|---|----------|--|
| Study Citation: | ECETOC, (1985). An assessment of the occurrence and effects of dialkyl ortho-phthalates in the environment. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 679967 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 0.71E3 ug/L | | | |
| CASRN and Test Material | Not Reported; BBP | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Hollifield, H.C. (1974). Rapid nephelometric estimate of water solubility of highly insoluble organic chemicals of environmental interest. Bull. Envir. Contam. Toxicol., 23, 579. no HERO ID.

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| Study Citation: | ECHA, (2012). Committee for Risk Assessment (RAC) Committee for Socio-economic Analysis (SEAC): Background document to the Opinion on the Annex XV dossier proposing restrictions on four phthalates: Annexes. |
| OECD Harmonized Template: | Water Solubility |
| HERO ID: | 7325405 |

| EXTRACTION | |
|---|------------------------------------|
| Parameter | Data |
| Water Solubility | 2.8 mg/L |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | none; not specified; not specified |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; liquid; NR |
| Temperature | 25-30°C |
| System | not specified |
| pH | not specified |
| Results Details Method | not specified |
| Standard Deviation Results | not specified |
| Results Details | not specified |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Source cited: EU RAR (2008b); but maybe EU RAR (2007). European Chemicals Bureau (2007). European Union, Risk Assessment Report, Butyl benzyl phthalate. Available at: http://esis.jrc.ec.europa.eu/doc/existing-chemicals/risk_assessment/REPORT/benzylbutylphthalatereport318.pdf

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|---|--|---|----------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 0.71 - 82.2 mg/L | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | collected from the literature | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Mackay, Shin and Ma (1994) Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals (volumes 2 and 3 are HERO ID 597912 and 5185256, respectively). Some values entered under HERO ID 679967 and 7401366.

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|---|--|---|--------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 0.71 - 82.2 mg/L | | | |
| CASRN and Test Material | 85-68-7; benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; experimental; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | collected from the literature | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Mackay, Shin and Ma (1994) Illustrated handbook of physical-chemical properties and environmental fate for organic chemicals (volumes 2 and 3 are HERO ID 597912 and 5185256, respectively). Some values entered under HERO ID 679967 and 7401366.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 5926420 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 0.67 - 2.4 mg/L | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | 25°C | | | |
| System | Not Reported | | | |
| pH | Not reported | | | |
| Results Details Method | Reported as 0.00067 to 0.0024 g/L at 25 C | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | 2 data points were reported in Reaxys; 2 values were reported at 0.00067 to 0.0024 g/L at standard temperature. | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb. 4; (1997); p. 667 - 749

| | |
|----------------------------------|---|
| Study Citation: | Hollifield, H. C. (1979). Rapid nephelometric estimate of water solubility of highly insoluble organic chemicals of environmental interest. Bulletin of Environmental Contamination and Toxicology 23(4-5):579-586. |
| OECD Harmonized Template: | Water Solubility |
| HERO ID: | 7401366 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| Water Solubility | 0.710 mg/L |
| CASRN and Test Material | Not Reported; Benzylbutyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | 0.5% or less stock in ethanol or acetone. Adjusted with same solvent until 0.5 -1.5 mL standard produced turbid suspension in 40 mL water.; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; Liquid; NR |
| Temperature | 24±2°C |
| System | Spectrophotofluorometer with a photomultiplier photometer, potted photomultiplier tube, and 150 W xenon arc lamp; test substance analyzed in standard 1-cm path length quartz fluorescence cuvette. |
| pH | Not reported |
| Results Details Method | Study performed at constant slit width, 3,2,2,3,5 slit arrangement. Excitation and emission monochromators set to 600 nm. |
| Standard Deviation Results | Not Reported |
| Results Details | 40 mL water, 1 mL gum tragacanth solution (stock 0.10 g/L in water) used to prevent suspensions, and test substance added by syringe at 0.1 mL/min were stirred by magnetic stirrer until first signs of turbidity. This was repeated with 0.1 mL increasing quantities of test substance to create 6-8 standards. Turbid solutions allowed to rest for 15 min, resuspended by stirring, and nephelometric measurements were recorded. Calibration curve extrapolated to blank prepared without test substance to determine solubility. |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|--|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is non-standard but is expected to be appropriate. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Citing METCALF, R.L. and P.Y. LU: "Environmental Distribution and Metabolic Fate of Key Industrial Pollutants and Pesticides in a Model Ecosystem," Research Report No. 69, University of Illinois Water Resources Center, 72 (1973).

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|---|--|---|----------|--|
| Study Citation: | Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 679985 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69 mg/L | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; If more than one manufacturer produced the individual PAE, the PAE product provided to us was an equal-proportion blend. | | | |
| Radiolabel, Source, State, and Purity | NR; Provided to Chemical Manufacturers’ Association by U.S. manufacturers.; NR; Each sample contained less than 1 % of non-PAE material, as determined by another laboratory. Notes: single isomer | | | |
| Temperature | 25°C | | | |
| System | Protocol was designed to meet or exceed the requirements of the EPA-recommended procedure stated in U.S. Environmental Protection Agency. 1979. TSCA premanufacture testing of new chemical substances: Water solubility. Fed. Reg. 44: 16253-16259. | | | |
| pH | Not reported | | | |
| Results Details Method | HPLC | | | |
| Standard Deviation Results | 0.15 | | | |
| Results Details | ASTM Type 2 water | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) and other physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | Standard test method used. |
| | Metric 4: | Reliability/Analytical Method | High | Protocol was designed to meet or exceed the requirements of the EPA-recommended procedure. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |
| Continued on next page ... | | | | |

...continued from previous page

| Study Citation: | Howard, P. H., Banerjee, S., Robillard, K. H. (1985). Measurement of water solubilities octanol-water partition coefficients and vapor pressures of commercial phthalate esters. Environmental Toxicology and Chemistry 4(5):653-662. | | |
|----------------------------------|---|-------------------|----------|
| OECD Harmonized Template: | Water Solubility | | |
| HERO ID: | 679985 | | |
| | | EVALUATION | |
| Domain | Metric | Rating | Comments |

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|---|--|---|----------|--|
| Study Citation: | Ishak, H., Mokbel, I., Saab, J., Stephan, J., Paricaud, P., Jose, J., Goutaudier, C. (2019). Experimental measurements and thermodynamic modelling of aqueous solubilities, octanol-water partition coefficients and vapor pressures of dimethyl phthalate and butyl benzyl phthalate. Journal of Chemical Thermodynamics 131:286-293. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 5433285 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 1.3E-7 - | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate-BBP | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | None; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; NR; 0.98 (Supplier purity) Notes: Purity checked by GC >0.99 | | | |
| Temperature | 298.15 K | | | |
| System | Test method: dynamic saturation method. | | | |
| pH | Not reported | | | |
| Results Details Method | HPLC-UV | | | |
| Standard Deviation Results | S = 3.95E-9, 95% confidence level | | | |
| Results Details | Reported as mean aqueous solubility in mole fraction = 1.30E-7; Measured at 0.1 MPa (ca. 750 mm Hg) | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | Low | Author indicates value may be underestimated as it deviates more than 10% from literature values. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is non-standard; great uncertainty was noted due to the difficulty of measuring very low aqueous solubility. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|---|--|---|---------------|---|
| Study Citation: | Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 807140 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 0.93 mg/L | | | |
| CASRN and Test Material | 85-68-7; butylbenzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; QSAR; Quantitative Structure-Property relationship model for estimation of water solubility | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: BBzP | | | |
| Temperature | not applicable | | | |
| System | QSPR model using the Lu index, which is based on the shortest distance matrix. | | | |
| pH | not applicable | | | |
| Results Details Method | Predictive model developed using Lu index: Log Sw = 8.2431 - 0.5718 (Lu) | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | n = 34; correlation coefficient (R) = 0.9869; standard error (SE) = 0.44; leave-one-out cross validation correlation coefficient (Rsv) = 0.9709; corresponding standarderrors (scv) = 0.47 | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | Uninformative | The QSPR model failed the standard error threshold of <0.3 and is therefore rated unacceptable. |
| Overall Quality Determination | | Medium | | |

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|---|--|---|----------|--|
| Study Citation: | Mueller, M., Klein, W. (1992). Comparative evaluation of methods predicting water solubility for organic compounds. Chemosphere 25(6):769-782. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 654554 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69 mg/L | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Calculation; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not reported | | | |
| System | Statistical estimation in relation to partition coefficients. | | | |
| pH | Not reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Reported as 8.61E-6 mol/L | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | Medium | Calculated data consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology’s objective is clear. |
| | Metric 4: | Reliability/Analytical Method | N/A | This matrix is not applicable to this calculated data. |
| Domain 3: Other | Metric 5: | Databases | N/A | This matrix is not applicable to this calculated data. |
| | Metric 6: | Models | High | The model had a defined, unambiguous endpoint and the model performance was known. |
| Overall Quality Determination | | High | | |

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| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Water Solubility |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Water Solubility | 2.69 mg/L |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 25°C |
| System | Not Reported |
| pH | Not reported |
| Results Details Method | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |

| EVALUATION | | | |
|----------------------------|---|--------|--|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical's physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a publicly available database that provides references to original sources. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Howard, P.H. et al. 1985. Environ Tox Chem 4: 653-661.

| | | | | |
|---|--|---------------|--|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69 mg/L | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | almost insoluble in distilled water | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. | |
| | Metric 2: Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. | |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. | |
| | Metric 4: Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. | |
| Domain 3: Other | Metric 5: Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. | |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. | |
| Overall Quality Determination | | Medium | | |

* Related References: data entered in HEROID: 679985 Howard et al (1985)

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|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.9 mg/L | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| Temperature | 20C | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: HEROID: 1337260 Gledhill et al (1980). An environmental safety assessment of butyl benzyl phthalate. Environ. Sci. Technol. 14, 301-305

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|---|---|---|----------|--|
| Study Citation: | NTP-CERHR, (2003). NTP-CERHR monograph on the potential human reproductive and developmental effects of butyl benzyl phthalate (BBP). | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 678590 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.7 mg/L | | | |
| CASRN and Test Material | 85-68-7; Butyl Benzyl Phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not Reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Reported as solubility in water: slight – 2.7 mg/L | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing CMA. Comments of the Chemical Manufacturers Association phthalate esters panel in response to request for public input on seven phthalate esters. FR Doc. 99-9484. Washington, DC: Chemical Manufacturers Association, 1999. No HERO ID.

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|---|--|---|----------|--|
| Study Citation: | SRC, (1983). Measurement of the water solubilities of phthalate esters (final report). | | | |
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 1316216 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69 - mg/L | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; experimental; Measured test compound solubility in water by HPLC | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | 25°C | | | |
| System | Samples shaken in distilled water, centrifuged and then analyzed | | | |
| pH | Not Reported | | | |
| Results Details Method | HPLC | | | |
| Standard Deviation Results | ±0.15 | | | |
| Results Details | The study reports that the experimental uncertainty exceeded that targeted in the SOP. Value reported based on curvilinear equation. Previously reported value = 2.83±0.14, value obtained by auditor = 2.88±0.14 (linear equation). | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Low | The study authors state that the experimental uncertainty exceeded that targeted in the SOP. |
| | Metric 4: | Reliability/Analytical Method | High | Data are obtained by accepted standard analytical methods, including, but not limited to OECD guidelines for physical-chemical properties or other developed standard. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

| Study Citation: | U.S. EPA, (2019). Chemistry Dashboard Information for Benzyl butyl phthalate. 85-68-7.. | | | |
|---|---|---|----------|--|
| OECD Harmonized Template: | Water Solubility | | | |
| HERO ID: | 5926148 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Water Solubility | 2.69 mg/L | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| pH | Not reported | | | |
| Results Details Method | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical’s physical/chemical properties. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available database that provides references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: PhysProp. Howard, PH et al. 1985.

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|----------------------------------|--|
| Study Citation: | NCBI, (2020). PubChem Compound Summary for CID 2347Benzyl butyl phthalate. |
| OECD Harmonized Template: | Flash Point |
| HERO ID: | 6629530 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Flash Point | 390 F |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR |
| System | Not reported |
| Standard Deviation Results | Not reported |
| Results Details | Not Reported |

| | | EVALUATION | | |
|----------------------------|-----------|---|----------|---|
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | Methodology was not reported in the secondary source. There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a secondary database with a reference to the original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

Medium

* Related References: National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

| | | | | |
|---|--|---|----------|---|
| Study Citation: | NCBI, (2020). PubChem Compound Summary for CID 2347Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Flash Point | | | |
| HERO ID: | 6629530 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Flash Point | 198 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| System | Not reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | Methodology was not reported in the secondary source. There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a secondary database with a reference to the original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: ILO International Chemical Safety Cards (ICSC)

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|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Flash Point |
| HERO ID: | 5926116 |

EXTRACTION

| Parameter | Data |
|---|----------------------------------|
| Flash Point | 390 F |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR |
| System | Closed cup |
| Standard Deviation Results | Not reported |
| Results Details | 199°C |

EVALUATION

| Domain | Metric | Rating | Comments |
|----------------------------|---|--------|--|
| Domain 1: Substance | Metric 1: Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: Databases | High | Data is from a secondary database with a reference to the original source. |
| | Metric 6: Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination**High**

* Related References: National Fire Protection Association; Fire Protection Guide to Hazardous Materials. 14TH Edition, Quincy, MA 2010, p. 325-18

| | | | | |
|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Flash Point | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Flash Point | 199 C | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Value added under HSDB (2015) HEROID: 5926116

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|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Flash Point | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Flash Point | 113 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Biosynth

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|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Flash Point | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Flash Point | 230 F | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: LabNetwork

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|---|--|---|----------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Flash Point | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Flash Point | 110 C | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Alfa Aesar

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|---|--|---|--------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Autoflammability | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Auto-flammability | 425 - C | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Value | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Bayer AG, 1999 Final GLP Report, Determination of Safety-Relevant Data of Unimoll BB (no HERO ID). Value also under HERO ID 6629530.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Autoflammability | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Auto-flammability | 425 - C | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; not specified; NR | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Value | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Citing Bayer AG, 1999 Final GLP Report, Determination of Safety-Relevant Data of Unimoll BB (no HERO ID). Value also under HERO ID 6629530.

| | | | | |
|---|--|---|----------|--|
| Study Citation: | NCBI, (2020). PubChem Compound Summary for CID 2347Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Autoflammability | | | |
| HERO ID: | 6629530 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Auto-flammability | 451 F | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR | | | |
| System | Not reported | | | |
| Standard Deviation Results | Not reported | | | |
| Results Details | Not reported | | | |
| Results Value | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: National Toxicology Program, Institute of Environmental Health Sciences, National Institutes of Health (NTP). 1992. National Toxicology Program Chemical Repository Database. Research Triangle Park, North Carolina.

| Study Citation: | NCBI, (2020). PubChem Compound Summary for CID 2347Benzyl butyl phthalate. | | | |
|---|--|---|--------|------------|
| OECD Harmonized Template: | Autoflammability | | | |
| HERO ID: | 6629530 | | | |
| Parameter | | EXTRACTION | | |
| Auto-flammability | | 425 C | | |
| CASRN and Test Material | | 85-68-7; Benzyl butyl phthalate | | |
| Confidentiality, Type, and Guideline | | None; Experimental; Not reported | | |
| Solvent, Reactivity, Storage, and Stability | | NR; NR; NR; NR | | |
| Radiolabel, Source, State, and Purity | | NR; NR; NR; NR | | |
| System | | Not reported | | |
| Standard Deviation Results | | Not reported | | |
| Results Details | | Not reported | | |
| Results Value | | Not Reported | | |
| Domain | | Metric | | EVALUATION |
| | | | | Rating |
| | | | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | | High |
| | Metric 2: | Appropriateness | | N/A |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | | Medium |
| | Metric 4: | Reliability/Analytical Method | | Low |
| Domain 3: Other | Metric 5: | Databases | | Medium |
| | Metric 6: | Models | | N/A |
| Overall Quality Determination | | | Medium | |

* Related References: ILO International Chemical Safety Cards (ICSC)

| | | | | |
|---|--|---|----------|--|
| Study Citation: | NTP, (1997). Toxicology and carcinogenesis studies of butyl benzyl phthalate (CAS No. 85-68-7) in F344/N rats (feed studies). National Toxicology Program Technical Report Series 458(1997):1-195. | | | |
| OECD Harmonized Template: | Autoflammability | | | |
| HERO ID: | 1239592 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Auto-flammability | 233 C | | | |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | None; NR; liquid; NR | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Value | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Verschueren, (1983) (page missing from document); Hawley's, (1987). 11th ed. (N.I. Sax and R.J. Lewis, Sr., Eds.), p. 184. Van Nostrand Reinhold, New York.; Sax and Lewis, (1989). Dangerous Properties of Industrial Materials. 7th. ed, pp. 41 1-412. Van Nostrand Reinhold, New York.

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|----------------------------------|--|
| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | Viscosity |
| HERO ID: | 5926420 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| Viscosity | 55 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 20°C |
| Test Conditions | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | At 20°C; 3 values were reported in Reaxys; 1 value was reported as 0.55 P at 20°C; 2 values were outside this range or measured at non-standard temperatures. |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: Data range determined from multiple primary sources in REAXYS.

| | | | | |
|---|--|---|--------|--|
| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. | | | |
| OECD Harmonized Template: | Refractive Index | | | |
| HERO ID: | 5926420 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Refractive Index | 1.5356 | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | 20°C | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| Parameter | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data’s inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a secondary database with a references to the peer-reviewed original source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | High | | |

* Related References: Fischer et al.; Pharmazeutische Zentralhalle; vol. 105; (1966); p. 73,74

| | |
|----------------------------------|---|
| Study Citation: | NLM, (2015). PubChem: Hazardous Substance Data Bank: Butyl benzyl phthalate, 85-68-7. |
| OECD Harmonized Template: | Refractive Index |
| HERO ID: | 5926116 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Refractive Index | 1.535 - 1.540 |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | 25°C |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |
| Results Details Methods | Not Reported |
| Parameter | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | Analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | Data is from a publicly available, peer-reviewed database that provides references to a recognized data collection. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: IARC. 1982. Monographs on the Evaluation of the Carcinogenic Risk of Chemicals to Humans. Geneva: World Health Organization, International Agency for Research on Cancer.

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|---|--|---|--------|---|
| Study Citation: | RSC, (2019). ChemSpider: Benzyl butyl phthalate. | | | |
| OECD Harmonized Template: | Refractive Index | | | |
| HERO ID: | 5926261 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Refractive Index | 1.54 | | | |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate | | | |
| Confidentiality, Type, and Guideline | None; Experimental; Not reported | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR | | | |
| Temperature | Not Reported | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| Parameter | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Medium | Data is from a publicly available secondary source with references to non-peer reviewed sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

* Related References: Alfa Aesar

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| Study Citation: | Cousins, I., Mackay, D. (2000). Correlating the physical–chemical properties of phthalate esters using the ‘three solubility’ approach. Chemosphere 41(9):1389-1399. |
| OECD Harmonized Template: | Henry's Law |
| HERO ID: | 4159647 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| Henry's Law | 0.205 Pa m ³ /mol |
| CASRN and Test Material | 85-68-7; Butylbenzyl phthalate |
| Confidentiality, Type, and Guideline | None; QSAR; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: BBP |
| Temperature | 25°C |
| pH | Not reported |
| System | Three solubility approach: a quantitative structure-property relationship; correlations between apparent-solubilities of liquid state compounds in air and water, and molecular structures used to estimate partition coefficient Kaw (air-water) |
| Standard Deviation Results | Not reported |
| Results Details | log Kaw = -4.08 |
| Results Details Methods | Not applicable |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|---|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | High | The methodology for producing the information is designed to answer a specific question, and the methodology's objective is clear. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | High | The model had a defined, unambiguous endpoint AND the model performance was known and r ² > 0.7, q ² > 0.5, and SE < 0.3. |

Overall Quality Determination

High

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|----------------------------------|--|
| Study Citation: | EC/HC, (2000). Canadian environmental protection act priority substances list assessment report: Butylbenzylphthalate. |
| OECD Harmonized Template: | Henry's Law |
| HERO ID: | 1333728 |

| EXTRACTION | |
|---|--|
| Parameter | Data |
| Henry's Law | 0.133 Pa-m3/mol |
| CASRN and Test Material | 85-68-7; Butylbenzylphthalate |
| Confidentiality, Type, and Guideline | no; not specified; Not Reported |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported |
| Temperature | Not Reported |
| pH | Not Reported |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Not Reported |
| Results Details Methods | Not Reported |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features (e.g., presence of certain functional groups) or other physical/chemical properties (e.g., if the physical state is described as a liquid, the substance should have a melting point below 25°C and a boiling point above 25°C) or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Medium | The analytical method is unknown but is likely to be appropriate based on the data's inclusion in a peer-reviewed/recognized database or other secondary source. |
| Domain 3: Other | Metric 5: | Databases | High | The information or data is from a recognized data collection/repository where data are peer-reviewed by experts in the field, are broadly available to the public for review and use OR includes references to the original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

High

* Related References: From: Lyman, W.J., W.F. Reehl and D.H. Rosenblatt.1982. Handbook on chemical property estimation methods. Environmental behaviour of organic compounds. McGraw-Hill, New York, N.Y. [cited in Howard, 1989] [HERO ID - 82189?]

| | | | | |
|---|--|---|----------|--|
| Study Citation: | ECJRC, (2008). European Union Summary Risk Assessment Report: Benzyl butyl phthalate (BBP) (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
| OECD Harmonized Template: | Henry’s Law | | | |
| HERO ID: | 2121719 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Henry’s Law | 0.176 - Pa.m3/mol | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; Calculation; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| pH | Not Reported | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

| Study Citation: | ECJRC, (2007). European Union Risk Assessment Report: Benzyl butyl phthalate (CAS No: 85-68-7, EINECS: 201-622-7). | | | |
|---|--|---|----------|--|
| OECD Harmonized Template: | Henry’s Law | | | |
| HERO ID: | 5348378 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Henry’s Law | 0.176 - Pa.m3/mol | | | |
| CASRN and Test Material | 85-68-7; Butyl benzyl phthalate | | | |
| Confidentiality, Type, and Guideline | No; Calculation; Not Reported | | | |
| Solvent, Reactivity, Storage, and Stability | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Radiolabel, Source, State, and Purity | Not Reported; Not Reported; Not Reported; Not Reported | | | |
| Temperature | Not Reported | | | |
| pH | Not Reported | | | |
| System | Not Reported | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Not Reported | | | |
| Results Details Methods | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Calculated data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | Medium | The data are from a source that is known but is missing elements required for High designation such as peer-review, public availability, or the inclusion of references to original sources. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |
| Overall Quality Determination | | Medium | | |

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|----------------------------------|--|
| Study Citation: | Elsevier, (2019). Reaxys: physical-chemical property data for butyl benzyl phthalate. CAS Registry Number: 85-68-7.. |
| OECD Harmonized Template: | Henry's Law |
| HERO ID: | 5926420 |

| EXTRACTION | |
|---|----------------------------------|
| Parameter | Data |
| Henry's Law | 7.61E-7 atm-m3/mol |
| CASRN and Test Material | 85-68-7; Benzyl butyl phthalate |
| Confidentiality, Type, and Guideline | None; Experimental; Not Reported |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | Not Reported; NR; NR; NR |
| Temperature | Not reported |
| pH | Not Reported |
| System | Not Reported |
| Standard Deviation Results | Not Reported |
| Results Details | Reported as 0.077108 Pa-m3/mol |
| Results Details Methods | Not Reported |

| | | EVALUATION | |
|----------------------------|-----------|---|----------|
| Domain | Metric | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High |
| | Metric 2: | Appropriateness | High |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium |
| | Metric 4: | Reliability/Analytical Method | Medium |
| Domain 3: Other | Metric 5: | Databases | High |
| | Metric 6: | Models | N/A |

Overall Quality Determination

High

* Related References: Staples, Charles A.; Peterson, Dennis R.; Parkerton, Thomas F.; Adams, William J.; Chemosphere; vol. 35; nb.4; (1997); p. 667 - 749

| | | | | |
|---|---|---|--------|--|
| Study Citation: | Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173. | | | |
| OECD Harmonized Template: | Henry's Law | | | |
| HERO ID: | 807140 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| Henry's Law | Not Reported | | | |
| CASRN and Test Material | 85-68-7; butylbenzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; QSAR; Quantitative Structure-Property relationship model for estimation of log Kaw | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: BBzP | | | |
| Temperature | Not Reported | | | |
| pH | Not Reported | | | |
| System | Kaw = S(A)/Sw where S(A) is the solubility in air and Sw is the solubility in water | | | |
| Standard Deviation Results | Not Reported | | | |
| Results Details | Log Kaw= -3.76 | | | |
| Results Details Methods | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | Medium | Modeled data compared well to other data. |
| Overall Quality Determination | | Medium | | |

| | |
|----------------------------------|--|
| Study Citation: | NICNAS, (2015). Priority existing chemical assessment report no. 40: Butyl benzyl phthalate. |
| OECD Harmonized Template: | Henry's Law |
| HERO ID: | 3664467 |

| EXTRACTION | |
|---|---|
| Parameter | Data |
| Henry's Law | 1.28X10 ⁻⁴ - kPa m ³ /mol |
| CASRN and Test Material | 85-68-7; butyl benzyl phthalate |
| Confidentiality, Type, and Guideline | No; not specified; NR |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: NR |
| Temperature | 25°C |
| pH | NR |
| System | Not Reported |
| Standard Deviation Results | NR |
| Results Details | NR |
| Results Details Methods | NR |

| EVALUATION | | | | |
|----------------------------|-----------|---|--------|--|
| Domain | Metric | | Rating | Comments |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | High | Measured data are consistent with the subject chemical substance structural features or other physical/chemical properties or behaviors. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | Medium | There is no indication that the methodology for producing the information was biased towards a particular product or outcome. |
| | Metric 4: | Reliability/Analytical Method | Low | The analytical method is unknown and there is no indication that a reliable method was used. |
| Domain 3: Other | Metric 5: | Databases | Low | Unable to confirm the value in the primary source. |
| | Metric 6: | Models | N/A | Rating of this factor is not applicable to this kind of information. |

Overall Quality Determination

Low

* Related References: Citing ChemIDplus and ECB (2007) European Union Risk Assessment Report (EU RAR) on benzyl butyl phthalate (BBP), HERO ID 2121719. However, different values were reported in these cited sources.

| | | | | |
|---|---|---|----------|--|
| Study Citation: | Lu, C. (2009). Prediction of environmental properties in water-soil-air systems for phthalates. Bulletin of Environmental Contamination and Toxicology 83(2):168-173. | | | |
| OECD Harmonized Template: | Other Properties | | | |
| HERO ID: | 807140 | | | |
| EXTRACTION | | | | |
| Parameter | Data | | | |
| CASRN and Test Material | 85-68-7; butylbenzyl phthalate | | | |
| Confidentiality, Type, and Guideline | none; QSAR; Quantitative Structure-Property relationship model for estimation of log Koa | | | |
| Solvent, Reactivity, Storage, and Stability | NR; NR; NR; NR | | | |
| Radiolabel, Source, State, and Purity | NR; NR; NR; NR Notes: BBzP | | | |
| Results Value | Log Koa = 8.98 | | | |
| Results Details | Koa = So/S(A) where So is solubility in octanol and S(A) is the solubility in air | | | |
| Results Remarks | Not Reported | | | |
| EVALUATION | | | | |
| Domain | Metric | Rating | Comments | |
| Domain 1: Substance | Metric 1: | Representativeness | High | Data are measured or estimated for the subject chemical substance. |
| | Metric 2: | Appropriateness | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 2: Test Reliability | Metric 3: | Reliability/Unbiased (Method Objectivity) | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 4: | Reliability/Analytical Method | N/A | Rating of this factor is not applicable to this kind of information. |
| Domain 3: Other | Metric 5: | Databases | N/A | Rating of this factor is not applicable to this kind of information. |
| | Metric 6: | Models | Medium | Modeled data compared well to other data. |
| Overall Quality Determination | | Medium | | |

List of Abbreviations and Acronyms for Data Quality Evaluation and Extraction Tables

| Term | Definition |
|---------------------------|---|
| ASTM | American Society for Testing and Materials |
| ATSDR | Agency for Toxic Substances and Disease Registry |
| atm | Atmospheres |
| atm · m ³ /mol | Atmospheres - cubic meters per mole |
| C | Celsius |
| CASRN | Chemical Abstract Service registry number |
| cP | Centipoise |
| CRC | CRC Handbook of Chemistry and Physics |
| DOE | U.S. Department of Energy |
| ECB | European Chemicals Bureau |
| EPA | Environmental Protection Agency |
| F | Fahrenheit |
| GC | Gas Chromatography |
| g/cm ³ | Grams per cubic centimeter |
| GLP | Good Laboratory Practice |
| HLC | Henry's Law Constant |
| HPV | High Production Volume |
| HSDB | Hazard Substance Data Bank |
| ILO | International Labour Organization |
| IPCS | International Programme on Chemical Safety |
| IUCLID | International Uniform Chemical Information Database |
| K | Kelvin |
| K _{oa} | Octanol-Air partition coefficient |
| K _{ow} | Octanol-Water partition coefficient |
| mg/L | Milligrams per Liter |
| mol | Mole |
| mmHg | Millimeters of Mercury |
| MS | Mass Spectrometry |
| N/A | Not Applicable |
| NICNAS | National Industrial Chemicals Notification and Assessment Scheme |
| NLM | National Library of Medicine |
| NR | Not Reported |
| OECD | Organisation for Economic Co-operation and Development |
| Pa (hPa) | Pascals (hectopascals; 1 hPa = 100 Pa) |
| pH | Negative base 10 Log of Hydrogen Ion (H ⁺) Concentration in Aqueous Solution |
| pK _a | Negative base 10 Log of Acid Dissociation Constant (K _a) |
| RIVM | National Institute for Public Health and the Environment (Dutch: Rijksinstituut voor Volksgezondheid en Milieu) |

Continued on next page ...

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| Term | Definition |
|-------------|-------------------------------|
| RSC | Royal Society of Chemistry |
| RT | Retention Time |
| SIDs | Screening Information Dataset |
| VP | Vapor Pressure |
| US or USA | United States of America |
| UV (UV-Vis) | Ultra Violet (UV-Visible) |
| WHO | World Health Organization |